

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Data pertaining to the chemical identity of cresols are listed in Table 3-1.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

The physical and chemical properties of cresols are presented in Tables 3-2.

TABLE 3-1. Chemical Identity of Cresols

| Characteristic | o-Cresol | p-Cresol | m-Cresol | o-, m-, and p-Cresol | References |
|-------------------------|---|---|--|---|---|
| Chemical name | o-Cresol | p-Cresol | m-Cresol | (o,m,p)-Cresol | CAS 1989 |
| Synonyms | 2-Methylphenol; 2-hydroxytoluene; o-cresylic acid | 4-Methylphenol; 4-hydroxytoluene; p-cresylic acid | 3-Methylphenol 3-hydroxytoluene; m-cresylic acid | Methylphenol; hydroxytoluene; cresylic acid | SANSS 1989; Chemline 1989; CAS 1989; HSDB 1989 |
| Trade names | No data | | | | |
| Chemical formula | C ₇ H ₈ O | C ₇ H ₈ O | C ₇ H ₈ O | C ₇ H ₈ O | CAS 1989 |
| Chemical structure | | | | Mixture of three previous isomers | |
| Identification numbers: | | | | | |
| CAS registry | 95-48-7 | 106-44-5 | 108-39-4 | 1319-77-3 | CAS 1989 |
| NIOSH RTECS | GO6300000 | GO6475000 | GO61250000 | GO5950000 | SANSS 1989 |
| EPA hazardous waste | FO04; U052 | FO04; U052 | FO04; U052 | FO04; U052 | HSDB 1989 |
| OHM/TADS | 7216652 | 7216653 | 7216651 | No data | OHM/TADS 1989 |
| DOT/UN/NA/IMCO shipping | UN 2076; IMO 6.1 | UN 2076; IMO 6.1 | UN 2076; IMO 6.1 | UN 2076; IMO 6.1 | HSDB 1989 |
| HSDB | 1813 | 1814 | 1815 | 250 | HSDB 1989 |
| NCI | No data | No data | No data | No data | |

CAS = Chemical Abstracts Service

DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Consultative Organization

EPA = Environmental Protection Agency

HSDB = Hazardous Substance Data Bank

NCI = National Cancer Institute

NIOSH = National Institute for Occupational Safety and Health

OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data Base

RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-2. Physical and Chemical Properties of Cresols

| Property | o-Cresol | m-Cresol | p-Cresol | Mixture of o-, p-, and m-cresol | References |
|--------------------------------|--|--|--|---------------------------------------|---|
| Molecular weight | 108.14 | 108.14 | 108.14 | 108.14 | Weast et al. 1988 |
| Color | White crystals darken with age | Colorless to yellowish | No data | Colorless, yellowish or pinkish | Sax and Lewis 1987; Windholz et al. 1983 |
| Physical state | Solid | Liquid | Solid | Liquid | Sax and Lewis 1987 |
| Melting point | 30.944°C | 12.22°C | 34.739°C | 11-35°C | Riddick et al. 1986; Sax and Lewis 1987 |
| Boiling point | | | | | |
| 1 atm | 191.004°C | 202.32°C | 201.94°C | 191-203°C | Riddick et al. 1986 |
| 10 mmHg | 74.9°C | 86°C | 85.7°C | | Weast et al. 1988; Sax and Lewis 1987 |
| Density (20°C) | 1.0273 g/mL | 1.0336 g/mL | 1.0178 g/mL | 1.030-1.047 g/mL | Weast et al. 1988 |
| Odor | Phenol-like | Phenol-like | Phenol-like | Phenol-like | Sax and Lewis 1987 |
| Odor threshold | | | | | |
| Water | No data | 0.00023 mg/L | No data | No data | Amoore and Hautula 1983 |
| Air | 0.65 ppm | 0.00028 ppm | 0.0455 ppm | No data | OHM/TADS 1989; Amoore and Hautula 1983 |
| Solubility | | | | | |
| Water at 25°C | 25,950 ppm | 22,700 ppm | 21,520 ppm | No data | Yalkowsky et al. 1987 |
| Organic solvents | Alcohol, ether, acetone, benzene, chloroform, alkali hydroxides(aq) | Alcohol, ether, acetone, benzene, chloroform, alkali hydroxides(aq) | Alcohol, ether, acetone, benzene, chloroform, alkali hydroxides(aq) | Alcohol, glycol, base | Weast et al. 1988; Sax and Lewis 1987; Windholz et al. 1983 |
| Partition coefficients | | | | | |
| Log octanol/water | 1.95 | 1.96 | 1.94 | No data | Hansch and Leo 1985 |
| Log K _{oc} | 1.03 | 1.54 | 1.69 | No data | Boyd 1982; Artiola- Fortuny and Fuller 1982 |
| Vapor pressure | | | | | |
| 25°C | 0.299 mmHg | 0.138 mmHg | 0.11 mmHg | No data | Chao et al. 1983; Daubert and Danner 1985 |
| Henry's law constant | | | | | |
| atm/m ³ -molecule | 1.2x10 ⁻⁶ | 8.65x10 ⁻⁷ | 7.92x10 ⁻⁷ | No data | Gaffney et al. 1987; Hine and Mookerjee 1975 |
| at 25°C | | (calculated from vapor pressure and water solubility) | | | |
| Flashpoint | 81°C | 86°C | 86°C | 82°C | Sax and Lewis 1987 |
| (closed cup) | | | | | |
| Flammability limits | | | | | |
| Air | 1.35 (lower) | 1.06-1.35% | 1.06-1.4% | No data | OHM/TADS 1989 |
| Conversion factors | | | | | |
| ppm (v/v) to mg/m ³ | | | | | |
| in air (20°C) | 4.50 | 4.50 | 4.50 | 4.50 | Verschueren 1983 |
| mg/m ³ to ppm (v/v) | | | | | |
| in air (20°C) | 0.22 | 0.22 | 0.22 | 0.22 | Verschueren 1983 |
| Bioconcentration factor | | | | | |
| log BCF | 1.25 (calculated from K _{ow}) | 1.30 | 1.24 (calculated from K _{ow}) | No data | Lyman et al. 1982; Freitag et al. 1985 |
| Explosive limits | No data | No data | No data | No data | |

